

Chapter 5

The Dirac Formalism and Hilbert Spaces

In the last chapter we introduced quantum mechanics using wave functions defined in position space. We identified the Fourier transform of the wave function in position space as a wave function in the wave vector or momentum space. Expectation values of operators that represent observables of the system can be computed using either representation of the wavefunction. Obviously, the physics must be independent whether represented in position or wave number space. P.A.M. Dirac was the first to introduce a representation-free notation for the quantum mechanical state of the system and operators representing physical observables. He realized that quantum mechanical expectation values could be rewritten. For example the expected value of the Hamiltonian can be expressed as

$$\int \psi^*(x) H_{op} \psi(x) dx = \langle \psi | H_{op} | \psi \rangle, \quad (5.1)$$

$$= \langle \psi | \varphi \rangle, \quad (5.2)$$

with

$$|\varphi\rangle = H_{op} |\psi\rangle. \quad (5.3)$$

Here, $|\psi\rangle$ and $|\varphi\rangle$ are vectors in a Hilbert-Space, which is yet to be defined. For example, complex functions of one variable, $\psi(x)$, that are square inte-

grable, i.e.

$$\int \psi^*(x) \psi(x) dx < \infty, \quad (5.4)$$

form the Hilbert-Space of square integrable functions denoted as L^2 . In Dirac notation this is

$$\int \psi^*(x) \psi(x) dx = \langle \psi | \psi \rangle. \quad (5.5)$$

Orthogonality relations can be rewritten as

$$\int \psi_m^*(x) \psi_n(x) dx = \langle \psi_m | \psi_n \rangle = \delta_{mn}. \quad (5.6)$$

As see above expressions look like a bracket he called the vector $|\psi_n\rangle$ a ket-vector and $\langle \psi_m|$ a bra-vector.

5.1 Hilbert Space

A Hilbert Space is a linear vector space, i.e. if there are two elements $|\varphi\rangle$ and $|\psi\rangle$ in this space the sum of the elements must also be an element of the vector space

$$|\varphi\rangle + |\psi\rangle = |\varphi + \psi\rangle. \quad (5.7)$$

The sum of two elements is commutative and associative

$$\text{Commutative : } |\varphi\rangle + |\psi\rangle = |\psi\rangle + |\varphi\rangle, \quad (5.8)$$

$$\text{Associative : } |\varphi\rangle + |\psi + \chi\rangle = |\varphi + \psi\rangle + |\chi\rangle. \quad (5.9)$$

The product of the vector with a complex quantity c is again a vector of the Hilbert-Space

$$c|\varphi\rangle \equiv |c\varphi\rangle. \quad (5.10)$$

The product between vectors and numbers is distributive

$$\text{Distributive : } c|\varphi + \psi\rangle = c|\varphi\rangle + c|\psi\rangle. \quad (5.11)$$

In short every linear combination of vectors in a Hilbert space is again a vector in the Hilbert space.

5.1.1 Scalar Product and Norm

There is a bilinear form defined by two elements of the Hilbert Space $|\varphi\rangle$ and $|\psi\rangle$, which is called a scalar product resulting in a complex number

$$\langle\varphi|\psi\rangle = a. \quad (5.12)$$

This scalar product obtained by exchanging the role of $|\varphi\rangle$ and $|\psi\rangle$ results in the complex conjugate number

$$\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^* = a^*. \quad (5.13)$$

The scalar product is distributive

$$\text{Distributive : } \langle\varphi|\psi_1 + \psi_2\rangle = \langle\varphi|\psi_1\rangle + \langle\varphi|\psi_2\rangle \quad . \quad (5.14)$$

$$\langle\varphi|c\psi\rangle = c\langle\varphi|\psi\rangle \quad . \quad (5.15)$$

And from Eq.(5.13) follows

$$\langle c\psi|\varphi\rangle = \langle\varphi|c\psi\rangle^* = c^*\langle\psi|\varphi\rangle \quad . \quad (5.16)$$

Thus if the complex number is pulled out from a bra-vector it becomes its complex conjugate. The bra- and ket-vectors are hermitian, or adjoint, to each other. The adjoint vector is denoted by the symbol⁺

$$(|\varphi\rangle)^+ = \langle\varphi| \quad , \quad (5.17)$$

$$(\langle\varphi|)^+ = |\varphi\rangle \quad . \quad (5.18)$$

The vector spaces of bra- and ket-vectors are dual to each other. To transform an arbitrary expression into its adjoint, one has to replace all operators and vectors by the adjoint operator or vector and in addition the order of the elements must be reversed. For example

$$(c|\varphi\rangle)^+ = c^*\langle\varphi| \quad , \quad (5.19)$$

$$\langle\varphi|\psi\rangle^+ = \langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle \quad . \quad (5.20)$$

This equation demands that a scalar product of a vector with itself is always real. Here, we even demand that it is positive

$$\langle\varphi|\varphi\rangle \geq 0, \quad \text{real} \quad . \quad (5.21)$$

The equal sign in Eq.(5.21) is only fulfilled for the null vector, which is defined by

$$|\varphi\rangle + 0 = |\varphi\rangle. \quad (5.22)$$

Note, we denote the null vector not with the symbol $|0\rangle$ but rather with the scalar 0. Because the symbol $|0\rangle$ is reserved for the ground state of a system.

If the scalar product of a vector with itself is always positive, Eq.(5.21), then one can derive from the scalar product the norm of a vector according to

$$\|\varphi\| = \sqrt{\langle\varphi|\varphi\rangle}. \quad (5.23)$$

For vectors that are orthogonal to each other we have

$$\langle\varphi|\psi\rangle = 0 \quad (5.24)$$

without having one of them be the null vector.

5.1.2 Vector Bases

The dimensions of a Hilbert space are countable, i.e. each dimension can be assigned a whole number and thereby all dimensions are referenced in a unique way with 1, 2, 3, A vector space that is a Hilbert space has the following additional properties.

Completeness:

If there is a sequence of vectors in a Hilbert space $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, |\varphi_4\rangle, \dots$ that fulfills Cauchy's convergence criterion then the limit vector $|\varphi\rangle$ is also an element of the Hilbert space. Cauchy's convergence criterion states that if $\|\varphi_n - \varphi_m\| < \varepsilon$, for some $n, m > N(\varepsilon)$ the sequence converges uniformly [2].

Separability:

The Hilbert space is separable. This indicates that for every element $|\varphi\rangle$ in the Hilbert space there is a sequence with $|\varphi\rangle$ as the limit vector.

Every vector in the Hilbert space can be decomposed into linear independent basis vectors $|\psi_n\rangle$. The number of basis vectors can be infinite

$$|\varphi\rangle = \sum_n c_n |\psi_n\rangle. \quad (5.25)$$

The components c_n of the vector $|\varphi\rangle$ with respect to the basis $|\psi_n\rangle$ are complex numbers denoted with index n . It is advantageous to orthonormalize the basis vectors

$$\langle\psi_n|\psi_m\rangle = \delta_{nm}. \quad (5.26)$$

The components of the vector $|\varphi\rangle$ can then be determined easily by

$$\langle\psi_m|\varphi\rangle = \sum_n c_n \langle\psi_m|\psi_n\rangle = \sum_n c_n \delta_{mn}, \quad (5.27)$$

or

$$c_m = \langle\psi_m|\varphi\rangle, \quad (5.28)$$

This leads to

$$|\varphi\rangle = \sum_n |\psi_n\rangle \langle\psi_n|\varphi\rangle. \quad (5.29)$$

5.2 Linear Operators in Hilbert Spaces

5.2.1 Properties of Linear Operators

An operator \mathbf{L} is defined as a mapping of a vector $|\varphi\rangle$ onto another vector $|\psi\rangle$ of the Hilbert space

$$\mathbf{L}|\varphi\rangle = |\psi\rangle. \quad (5.30)$$

A linear operator \mathbf{L} has the property that it maps a linear combination of input vectors to the linear combination of the corresponding maps

$$\begin{aligned} \mathbf{L}(a|\varphi_1\rangle + b|\varphi_2\rangle) &= (a\mathbf{L}|\varphi_1\rangle + b\mathbf{L}|\varphi_2\rangle) \\ &= a|\psi_1\rangle + b|\psi_2\rangle, \text{ for } a, b \in \mathbb{C}. \end{aligned} \quad (5.31)$$

The sum of two linear operators is defined as

$$(\mathbf{L} + \mathbf{M})|\varphi\rangle = \mathbf{L}|\varphi\rangle + \mathbf{M}|\varphi\rangle. \quad (5.32)$$

And the product of two operators is defined as

$$\mathbf{L}\mathbf{M}|\varphi\rangle = \mathbf{L}(\mathbf{M}|\varphi\rangle). \quad (5.33)$$

The null element and 1-element of the operators is denoted as $\mathbf{0}$, and $\mathbf{1}$. Often we will not bold face these operators, especially in products, where a

scalar has the same meaning. The two operators are defined by their action on arbitrary vectors of the Hilbert space

$$\mathbf{0}|\varphi\rangle = 0, \forall |\varphi\rangle, \quad (5.34)$$

$$\mathbf{1}|\varphi\rangle = |\varphi\rangle, \forall |\varphi\rangle \quad (5.35)$$

In generally, the multiplication of two operators is not commutative

$$\mathbf{L M} |\varphi\rangle \neq \mathbf{M L} |\varphi\rangle, \forall |\varphi\rangle, \quad (5.36)$$

or in short

$$\mathbf{L M} \neq \mathbf{M L}. \quad (5.37)$$

The expression

$$[\mathbf{L}, \mathbf{M}] = \mathbf{L M} - \mathbf{M L} \quad (5.38)$$

is therefore called the commutator between \mathbf{L} and \mathbf{M} . If $[\mathbf{L}, \mathbf{M}] = \mathbf{0}$, the operators commute. The following rules for commutators apply:

$$[\mathbf{L}, \mathbf{M}] = -[\mathbf{M}, \mathbf{L}] , \quad (5.39)$$

$$[\mathbf{L}, \mathbf{L}] = \mathbf{0} , \quad (5.40)$$

$$[\mathbf{L}, \mathbf{1}] = \mathbf{0} , \quad (5.41)$$

$$[\mathbf{L}, \mathbf{L}^{-1}] = \mathbf{0} , \quad (5.42)$$

$$[\mathbf{L}, a\mathbf{M}] = a [\mathbf{L}, \mathbf{M}] , \quad (5.43)$$

$$[\mathbf{L}_1 + \mathbf{L}_2, \mathbf{M}] = [\mathbf{L}_1, \mathbf{M}] + [\mathbf{L}_2, \mathbf{M}] , \quad (5.44)$$

$$[\mathbf{L}, \mathbf{M}] = -[\mathbf{M}, \mathbf{L}] \quad (5.45)$$

$$[\mathbf{L}_1\mathbf{L}_2, \mathbf{M}] = [\mathbf{L}_1, \mathbf{M}] \mathbf{L}_2 + \mathbf{L}_1 [\mathbf{L}_2, \mathbf{M}] , \quad (5.46)$$

$$[\mathbf{M}, \mathbf{L}_1\mathbf{L}_2] = [\mathbf{M}, \mathbf{L}_1] \mathbf{L}_2 + \mathbf{L}_1 [\mathbf{M}, \mathbf{L}_2] . \quad (5.47)$$

Often the anticommutator is also used. It is defined as

$$[\mathbf{L}, \mathbf{M}]_+ = \mathbf{L M} + \mathbf{M L} . \quad (5.48)$$

If $[\mathbf{L}, \mathbf{M}]_+ = \mathbf{0}$, the operators are called anti-commuting.

5.2.2 The Dyadic Product

Two vectors in the Hilbert space can not only be used to build a scalar product but rather what is called a dyadic product, which is an operator

$$|\alpha\rangle\langle\beta|. \quad (5.49)$$

The dyadic product is the formal product between a ket- and a bra-vector. If applied to a vector, it projects the vector onto the state $|\beta\rangle$ and generates a new vector in parallel to $|\alpha\rangle$ with a magnitude equal to the projection

$$|\alpha\rangle\langle\beta|\psi\rangle = \langle\beta|\psi\rangle|\alpha\rangle. \quad (5.50)$$

As we have seen from Eq.(5.29), if $|\psi_n\rangle$ built a complete orthonormal basis, then

$$|\varphi\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\varphi\rangle, \quad \forall |\varphi\rangle, \quad (5.51)$$

Eq.(5.35) implies

$$\mathbf{1} = \sum_n |\psi_n\rangle\langle\psi_n|. \quad (5.52)$$

When applied to an operator from the left and right side

$$\begin{aligned} \mathbf{1} \mathbf{L} \mathbf{1} &= \sum_m |\psi_m\rangle\langle\psi_m| \left(\sum_n \mathbf{L} |\psi_n\rangle\langle\psi_n| \right) \\ &= \sum_m \sum_n L_{mn} |\psi_m\rangle\langle\psi_n| \end{aligned} \quad (5.53)$$

with the matrix elements

$$L_{mn} = \langle\psi_m|\mathbf{L}|\psi_n\rangle. \quad (5.54)$$

The matrix elements L_{mn} represent the operator in the chosen base $|\psi_n\rangle$. Once we choose a base and represent vectors and operators in term of this base, the components of the vector and the operator can be collected in a column vector and a matrix. The table below shows a comparison between a representation based on Hilbert space vectors and operators in term of vectors and matrices in an euclidian vector space. Initially matrix mechanics was

developed by Heisenberg independently from Schroedingers wave mechanics. The Dirac representation in terms of bra- and ket-vectors unifies them and shows that both forms are isomorph

Ket-vector	Column vector
$ \varphi_a\rangle = \sum_n a_n \psi_n\rangle$	$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$
Bra-vector	Row vector
$\langle\varphi = \sum_n a_n^* \langle\psi_n $	$(a_1^* \ a_2^* \ \cdots)$
Inner product	Scalar product
$\langle\varphi_a \varphi_b\rangle = \sum_m \sum_n a_m^* b_n \langle\psi_m \psi_n\rangle$	$(a_1^* \ a_2^* \ \cdots) \cdot \begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix}$
$= \sum_n a_n^* b_n$	$= a_1^* b_1 + a_2^* b_2 + \cdots$
Operator	Matrix
$L = \sum_{m,n} L_{mn} \psi_m\rangle \langle\psi_n $	$\begin{pmatrix} L_{11} & L_{12} & \cdots \\ L_{21} & L_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$
Dyadic Product	
$ \varphi_a\rangle \langle\varphi_b = \sum_{m,n} a_m b_n^* \psi_m\rangle \langle\psi_n $	$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \cdot (b_1^* \ b_2^* \ \cdots) =$
	$= \begin{pmatrix} a_1 b_1^* & a_1 b_2^* & \cdots \\ a_2 b_1^* & a_2 b_2^* & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$

5.2.3 Special Linear Operators

5.2.4 Inverse Operators

The operator inverse to a given operator \mathbf{L} is denoted as \mathbf{L}^{-1}

$$\forall |\varphi\rangle, |\psi\rangle = \mathbf{L} |\varphi\rangle \implies |\varphi\rangle = \mathbf{L}^{-1} |\psi\rangle, \quad (5.55)$$

which leads to

$$\mathbf{L}\mathbf{L}^{-1} = \mathbf{1} \quad (5.56)$$

The inverse of a product is the product of the inverse in inverse order

$$(\mathbf{M}\mathbf{L})^{-1} = \mathbf{L}^{-1}\mathbf{M}^{-1} \quad (5.57)$$

5.2.5 Adjoint or Hermitian Conjugate Operators

The adjoint (hermitian conjugate) operator \mathbf{L}^+ is defined by

$$\langle \varphi | \mathbf{L}^+ | \psi \rangle = (\langle \psi | \mathbf{L} | \varphi \rangle)^* = \langle \psi | \mathbf{L} | \varphi \rangle^*, \quad (5.58)$$

here $|\varphi\rangle$ and $|\psi\rangle$ are arbitrary vectors in a Hilbert space. Note, that if the adjoint of an expression is formed, each component gets conjugated and the order is reversed. For example

$$(\mathbf{L} | \varphi \rangle)^+ = \langle \varphi | \mathbf{L}^+, \quad (5.59)$$

$$(\mathbf{L}^+ | \varphi \rangle)^+ = \langle \varphi | \mathbf{L} \quad (5.60)$$

If

$$|\mathbf{L}\varphi\rangle = \mathbf{L} |\varphi\rangle. \quad (5.61)$$

there is

$$\langle \mathbf{L}\varphi | = \langle \varphi | \mathbf{L}^+ \quad (5.62)$$

and

$$\langle \psi | \mathbf{L} | \varphi \rangle = \langle \psi | \mathbf{L}\varphi \rangle = \langle \mathbf{L}^+ \psi | \varphi \rangle \quad (5.63)$$

The matrix elements of the adjoint operator are

$$L_{mn}^+ = \langle \psi_m | \mathbf{L}^+ | \psi_n \rangle = \langle \psi_n | \mathbf{L} | \psi_m \rangle = L_{nm}^* \quad (5.64)$$

The following rules apply to adjoint operators

$$(\mathbf{L}^+)^+ = \mathbf{L}, \quad (5.65)$$

$$(a\mathbf{L})^+ = a^*\mathbf{L}^+, \quad (5.66)$$

$$(\mathbf{L} + \mathbf{M})^+ = \mathbf{L}^+ + \mathbf{M}^+, \quad (5.67)$$

$$(\mathbf{L} \mathbf{M})^+ = \mathbf{M}^+ \mathbf{L}^+. \quad (5.68)$$

5.2.6 Hermitian Operators

If the adjoint operator \mathbf{L}^+ is identical to the operator itself, then we call the operator hermitian

$$\mathbf{L} = \mathbf{L}^+. \quad (5.69)$$

Hermitian operators have real expected values. *Observables are represented by hermitian operators.*

5.2.7 Unitary Operators

If the inverse of an operator \mathbf{U} is the adjoint operator

$$\mathbf{U}^{-1} = \mathbf{U}^+, \quad (5.70)$$

then this operator is called a unitary operator and

$$\mathbf{U}^+ \mathbf{U} = \mathbf{U} \mathbf{U}^+ = \mathbf{1}. \quad (5.71)$$

If the operator \mathbf{U} is unitary and \mathbf{H} is a hermitian operator, then the product $\mathbf{U} \mathbf{H} \mathbf{U}^{-1}$ is also a hermitian operator.

$$(\mathbf{U} \mathbf{H} \mathbf{U}^{-1})^+ = (\mathbf{U}^{-1})^+ \mathbf{H}^+ \mathbf{U}^+ = \mathbf{U} \mathbf{H} \mathbf{U}^{-1}. \quad (5.72)$$

5.2.8 Projection Operators

The dyadic product

$$\mathbf{P}_n = |\psi_n\rangle \langle \psi_n|, \quad (5.73)$$

is a projection operator \mathbf{P}_n that projects a given state $|\varphi\rangle$ onto the unit vector $|\psi_n\rangle$

$$\mathbf{P}_n |\varphi\rangle = |\psi_n\rangle \langle \psi_n | \varphi \rangle. \quad (5.74)$$

If $|\varphi\rangle$ is represented in the orthonormal base $|\psi_n\rangle$

$$|\varphi\rangle = \sum_n c_n |\psi_n\rangle, \quad (5.75)$$

we obtain

$$\mathbf{P}_n |\varphi\rangle = c_n |\psi_n\rangle. \quad (5.76)$$

By construction, projection operators are hermitian operators. Besides operators that project on vectors, there are also operators that project on subspaces of the Hilbert space

$$\mathbf{P}_U = \sum_U |\psi_n\rangle \langle \psi_n|. \quad (5.77)$$

Here, the orthonormal vectors $|\psi_n\rangle$ span the sub-space U . Projection operators are idempotent

$$\mathbf{P}_n^k = \mathbf{P}_n, \text{ for } k > 1. \quad (5.78)$$

5.3 Eigenvalues of Operators

In chapter 4, we studied the eigenvalue problem of differential operators. Here, we want to formulate the eigenvalue problem of operators in a Hilbert space. An operator \mathbf{L} in a Hilbert space with eigenvectors $|\psi_n\rangle$ fulfills the equations

$$\mathbf{L}|\psi_n\rangle = L_n|\psi_n\rangle, \quad (5.79)$$

with eigenvalues L_n . If there exist several different eigenvectors to the same eigenvalue L_n , this eigenvalue is called degenerate. For example, the energy eigenfunctions of the hydrogen atom are degenerate with respect to the indices l and m . The set of all eigenvalues is called the eigenvalue spectrum of the operator \mathbf{L} . As shown earlier the eigenvalues of hermitian operators are real and the eigenvectors to different eigenvalues are orthogonal to each other, because

$$\langle \psi_m | \mathbf{L} | \psi_n \rangle = L_n \langle \psi_m | \psi_n \rangle = L_m \langle \psi_m | \psi_n \rangle, \quad (5.80)$$

or

$$(L_n - L_m) \langle \psi_m | \psi_n \rangle = 0. \quad (5.81)$$

If the eigenvectors of the operator \mathbf{L} form a complete base of the Hilbert space, the operator \mathbf{L} is represented in this base by a diagonal matrix

$$L_{mn} = \langle \psi_m | \mathbf{L} | \psi_n \rangle = L_n \langle \psi_m | \psi_n \rangle = L_n \delta_{mn} \quad (5.82)$$

The operator can then be written in its spectral representation

$$\mathbf{L} = \sum_n L_n |\psi_n\rangle \langle \psi_n| = \sum_n L_n P_n. \quad (5.83)$$

5.4 Eigenvectors of Commuting Operators

Two operators, \mathbf{A} and \mathbf{B} , that commute with each other have a common set of eigenvectors. To prove this theorem, we assume that the eigenvalue spectrum of the operator \mathbf{A} is non degenerate. The eigenvectors and eigenvalues of operator \mathbf{A} are $|\psi_n\rangle$ and A_n , respectively

$$\mathbf{A}|\psi_n\rangle = A_n|\psi_n\rangle . \quad (5.84)$$

Using

$$[\mathbf{A}, \mathbf{B}] = 0, \quad (5.85)$$

we find

$$\begin{aligned} \langle\psi_m|\mathbf{A}\mathbf{B} - \mathbf{B}\mathbf{A}|\psi_n\rangle &= 0 & (5.86) \\ \langle\psi_m|\mathbf{A}\left(\sum_n|\psi_n\rangle\langle\psi_n|\right)\mathbf{B} - \mathbf{B}\mathbf{A}|\psi_n\rangle &= 0 \\ (A_m - A_n)\langle\psi_m|\mathbf{B}|\psi_n\rangle &= (A_m - A_n)B_{mn} = 0 . \end{aligned}$$

Since the eigenvalues are assumed to be not degenerate, i.e. $A_m \neq A_n$, the matrix B_{mn} must be diagonal, which means that the vector $|\psi_n\rangle$ has also to be an eigenvector of operator \mathbf{B} . If the eigenvalues are degenerate, one can always choose, in the sub-space that belongs to the degenerate eigenvalue, a base that are also eigenvectors of \mathbf{B} . The operator \mathbf{B} thus eventually has no degeneracies in this sub-space and therefore, the eigenvalues of \mathbf{B} may help to uniquely characterize the set of joint eigenvectors.

Also the reverse is true. If two operators have a joint system of eigenvectors, they commute. This is easy to see from the spectral representation of both operators.

Example: We define the parity operator P_x which, when applied to a wave function of a particle in one dimension $\psi(x)$, changes the sign of the position x

$$P_x\psi(x) = \psi(-x). \quad (5.87)$$

The Hamiltonian of a particle in an inversion symmetric potential $V(x)$, i.e.

$$V(x) = V(-x), \quad (5.88)$$

commutes with the parity operator. Then the eigenfunctions of the Hamiltonian are also eigenfunctions of the parity operator. The eigenfunctions of the

parity operator are the symmetric or antisymmetric functions with eigenvalues 1 and -1 , respectively. Therefore, the eigenfunctions of a Hamiltonian with symmetric potential has symmetric and antisymmetric eigenfunctions, see box potential and harmonic oscillator potential.

5.5 Complete System of Commuting Operators

In the case of the hydrogen atom, we had to use three quantum numbers n, l , and m to characterize the energy eigenfunctions completely. Without proof, the indices l and m characterize the eigenvalues of the square of the angular momentum operator \vec{L}^2 , and of the z -component of the angular momentum L_z with eigenvalues $l(l+1)\hbar^2$ and $m\hbar$, respectively. One can show, that the Hamilton operator of the hydrogen atom, the square of the angular momentum operator and the z -component of the angular momentum operator commute with each other and build a complete system of commuting operators (CSCO), whose eigenvalues enable a unique characterization of the energy eigenstates of the hydrogen atom.

5.6 Product Space

Very often in quantum mechanics one deals with interacting systems, for example system A and system B . The state space of each isolated system is Hilbert space H_A and Hilbert space H_B spanned by a complete base $|\psi_n\rangle_A$ and $|\psi_n\rangle_B$, respectively. \mathbf{L}_A and \mathbf{M}_B are operators on each of the Hilbert spaces of the individual systems. The Hilbert space of the total system is the product space

$$H = H_A \otimes H_B. \quad (5.89)$$

The vectors in this Hilbert space are given by the direct product of the individual vectors and one could choose as a base in the product space

$$|\chi_{nm}\rangle = |\psi_n\rangle_A \otimes |\psi_m\rangle_B = |\psi_n\rangle_A |\psi_m\rangle_B. \quad (5.90)$$

Operators that only act on system A can be extended to operate on the product space by

$$\mathbf{L} = \mathbf{L}_A \otimes \mathbf{1}_B. \quad (5.91)$$

or similar for operators acting on system B

$$\mathbf{M} = \mathbf{1}_A \otimes \mathbf{M}_B. \quad (5.92)$$

The product of both operators is then

$$\mathbf{LM} = \mathbf{L}_A \otimes \mathbf{M}_B. \quad (5.93)$$

An operator in this product space acts on a vector in the following way

$$\mathbf{LM} |\chi_{nm}\rangle = \mathbf{L} |\psi_n\rangle_A \otimes \mathbf{M} |\psi_m\rangle_B. \quad (5.94)$$

Since, the vectors $|\psi_n\rangle_A$ and $|\psi_m\rangle_B$ build a complete base for system A and B , respectively, the product vectors in Eq.(5.90) build a complete base for the interacting system and each state can be written in terms of this base

$$|\chi\rangle = \sum_{m,n} a_{mn} |\chi_{nm}\rangle = \sum_{m,n} a_{mn} |\psi_n\rangle_A \otimes |\psi_m\rangle_B. \quad (5.95)$$

5.7 Quantum Dynamics

In chapter 4, we derived the Schroedinger Equation in the x -representation. The stationary Schroedinger Equation was written as an eigenvalue problem to the Hamiltonian operator, which was then a differential operator. With the Dirac formulation we can rewrite these equations without referring to a special representation.

5.7.1 Schroedinger Equation

In the Dirac notation the Schroedinger Equation is

$$j\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \mathbf{H} |\Psi(t)\rangle. \quad (5.96)$$

\mathbf{H} is the Hamiltonian operator; it determines the dynamics of the quantum system.

$$\mathbf{H} = \frac{\tilde{\mathbf{p}}^2}{2m} + \mathbf{V}(\tilde{\mathbf{x}}). \quad (5.97)$$

The Hamiltonian operator is the generator of motion in a quantum system. Here $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{x}}$ and functions of them are operators in the Hilbert space. $|\Psi(t)\rangle$ is the Hilbert space vector describing fully the system's quantum state at time t . When looking for states that have a harmonic temporal behaviour

$$|\Psi(t)\rangle = e^{jE_n t/\hbar} |\psi_n\rangle, \quad (5.98)$$

we obtain the stationary Schroedinger Equation

$$\mathbf{H} |\psi_n\rangle = E_n |\psi_n\rangle, \quad (5.99)$$

that determines the energy eigenstates of the system. If the $|\psi_n\rangle$ build a complete basis of the Hilbert space, H , the system is dynamically evolving, the most general time dependent solution of the Schroedinger Equation is then a superposition of all energy eigenstates

$$|\Psi(t)\rangle = \sum_n a_n e^{jE_n t/\hbar} |\psi_n\rangle. \quad (5.100)$$

5.7.2 Schroedinger Equation in x-representation

We can return to wave mechanics by rewriting the abstract Schroedinger Equation in the eigenbase $|x\rangle$ of the position operator. For simplicity in notation, we only consider the one dimensional case and define that there exists the following eigenvectors

$$\mathbf{x} |x'\rangle = x' |x'\rangle, \quad (5.101)$$

with the orthogonality relation

$$\langle x | x'\rangle = \delta(x - x'). \quad (5.102)$$

Note, since the position operator has a continuous spectrum of eigenvalues the orthogonality relation is a dirac delta function rather than a delta-symbol. The completeness relation using this base is expressed in the unity operator

$$\mathbf{1} = \int |x'\rangle \langle x'| dx', \quad (5.103)$$

rather than a sum as in Eq.(5.52). Inserting this unity operator in the Schroedinger Equation (5.96) and projecting from the left with $\langle x|$, we obtain

$$j \hbar \frac{\partial}{\partial t} \langle x | \Psi(t)\rangle = \langle x | \mathbf{H} \int |x'\rangle \langle x'| \Psi(t)\rangle dx'. \quad (5.104)$$

The expression $\langle x | \Psi(t) \rangle$ is the probability amplitude that a position measurement on the system in state $|\Psi(t)\rangle$ yields the value x , which is precisely the meaning of the wave function

$$\Psi(x, t) = \langle x | \Psi(t) \rangle \quad (5.105)$$

in chapter 4. Using the eigenvalue property of the states and the orthogonality relations we obtain from Eq.(5.104)

$$j \hbar \frac{\partial}{\partial t} \Psi(x, t) = H(x, p = \frac{\hbar}{j} \frac{\partial}{\partial x}) \Psi(x, t). \quad (5.106)$$

5.7.3 Canonical Quantization

Thus the dynamics of a quantum system is fully determined by its Hamiltonian operator. The Hamiltonian operator is usually derived from the classical Hamilton function according to the Hamilton-Jacobi formulation of Classical Mechanics [3]. The classical Hamilton function $H(\{q_i\}, \{p_i\})$ is a function of the position coordinates of a particle x_i or generalized coordinates q_i and the corresponding momentum coordinates p_i . The classical equations of motion are found by

$$\dot{q}_i(t) = \frac{\partial}{\partial p_i} H(\{q_i\}, \{p_i\}), \quad (5.107)$$

$$\dot{p}_i(t) = -\frac{\partial}{\partial q_i} H(\{q_i\}, \{p_i\}). \quad (5.108)$$

In quantum mechanics the Hamiltonian function and the position and momentum coordinates become operators and quantization is achieved by imposing on position and momentum operators that are related to the same degree of freedom, for example the x -coordinate of a particle and the associate momentum p_x , canonical commutation relations

$$H(\{q_i\}, \{p_i\}) \Rightarrow \mathbf{H}(\{\mathbf{q}_i\}, \{\mathbf{p}_i\}), \quad (5.109)$$

$$[\mathbf{q}_i, \mathbf{p}_j] = j \hbar \delta_{ij}. \quad (5.110)$$

Imposing this commutation relation implies that position and momentum related to one degree of freedom can not be measured simultaneously with arbitrary precision and Heisenberg's uncertainty relation applies to the possible states the system can take on.

5.7.4 Schroedinger Picture

In the Schroedinger picture the quantum mechanical state of the system is evolving with time. If there is no explicit time dependence in the operators then the operators stay time independent. The Schroedinger Equation (5.96)

$$j\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \mathbf{H} |\Psi(t)\rangle, \quad (5.111)$$

plus the initial state

$$|\Psi(t=0)\rangle = |\Psi(0)\rangle, \quad (5.112)$$

uniquely determine the dynamics of the system. The evolution of the quantum state vector can be described as a mapping of the initial state by a time evolution operator.

$$|\Psi(t)\rangle = \mathbf{U}(t) |\Psi(0)\rangle. \quad (5.113)$$

If this solution is substituted into the Schroedinger Equation (5.111) it follows that the time evolution operator has to obey the equation

$$j\hbar \frac{\partial}{\partial t} \mathbf{U}(t) = \mathbf{H} \mathbf{U}(t). \quad (5.114)$$

For a time independent Hamiltonian Operator the formal integration of this equation is

$$\mathbf{U}(t) = \exp[-j\mathbf{H}t/\hbar]. \quad (5.115)$$

The time evolution operator is unitary

$$\mathbf{U}^{-1}(t) = \mathbf{U}^+(t), \quad (5.116)$$

because the Hamiltonian operator is hermitian, and therefore the norm of an initial state is preserved. The initial value for the time evolution operator is

$$\mathbf{U}(t=0) = \mathbf{1}. \quad (5.117)$$

The expected value of an arbitrary operator \mathbf{A} is given by

$$\langle \Psi(t) | \mathbf{A} | \Psi(t) \rangle = \langle \Psi(0) | \mathbf{U}^+(t) \mathbf{A} \mathbf{U}(t) | \Psi(0) \rangle. \quad (5.118)$$

5.7.5 Heisenberg Picture

Since the physically important quantities are the expected values, i.e. the outcome of experiments, Eq.(5.118) can be used to come up with an alternative formulation of quantum mechanics. In this formulation, called the Heisenberg picture, the operators are evolving in time according to

$$\mathbf{A}_H(t) = \mathbf{U}^+(t)\mathbf{A}\mathbf{U}(t), \quad (5.119)$$

and the state of the system is time independent and equal to its initial state

$$|\Psi_H(t)\rangle = |\Psi_S(0)\rangle. \quad (5.120)$$

Clearly an expected value for a time dependent operator using the Heisenberg state (5.120) is identical with Eq.(5.116).

This is identical to describing a unitary process in an euclidian vector space. Scalar products between vectors are preserved, if all vectors are undergoing a unitary transformation, i.e. a rotation for example. An alternative description is that the vectors are time independent but the coordinate system rotates in the opposite direction. When the coordinate system changes, the operators described in the time dependent coordinate system become time dependent themselves.

From the definition of the time evolution operator we find immediately an equation of motion for the time dependent operators of the Heisenberg picture

$$\begin{aligned} j\hbar \frac{\partial \mathbf{A}_H(t)}{\partial t} &= \left(j\hbar \frac{\partial \mathbf{U}^+(t)}{\partial t} \right) \mathbf{A}_S \mathbf{U}(t) + \mathbf{U}^+(t) \mathbf{A}_S \left(j\hbar \frac{\partial \mathbf{U}(t)}{\partial t} \right) \\ &+ \mathbf{U}^+(t) \left(j\hbar \frac{\partial \mathbf{A}_S}{\partial t} \right) \mathbf{U}(t) \end{aligned} \quad (5.121)$$

$$\begin{aligned} j\hbar \frac{\partial \mathbf{A}_H(t)}{\partial t} &= -\mathbf{U}^+(t) \mathbf{H}^+ \mathbf{A}_S \mathbf{U}(t) + \mathbf{U}^+(t) \mathbf{A}_S \mathbf{H} \mathbf{U}(t) \\ &+ \mathbf{U}^+(t) \left(j\hbar \frac{\partial \mathbf{A}_S}{\partial t} \right) \mathbf{U}(t) \end{aligned} \quad (5.122)$$

Using the relation $\mathbf{U}^+(t)\mathbf{U}(t) = \mathbf{U}(t)\mathbf{U}^+(t) = \mathbf{1}$ and inserting it between the Hamiltonian operator and the operator \mathbf{A} , we finally end up with the

Heisenberg equations of motion for the Heisenberg operators

$$j\hbar \frac{\partial}{\partial t} \mathbf{A}_H(t) = -\mathbf{H}_H \mathbf{A}_H + \mathbf{A}_H \mathbf{H}_H + j\hbar \left(\frac{\partial \mathbf{A}}{\partial \mathbf{t}} \right)_H \quad (5.123)$$

$$= [\mathbf{A}_H, \mathbf{H}_H] + j\hbar \left(\frac{\partial \mathbf{A}}{\partial \mathbf{t}} \right)_H \quad (5.124)$$

with

$$\mathbf{H}_H = \mathbf{U}^\dagger(t) \mathbf{H}_S \mathbf{U}(t) \quad (5.125)$$

$$= \mathbf{H}_S \text{ for conservative systems, i.e. } \mathbf{H}_S \neq \mathbf{H}_S(t) \quad (5.126)$$

Note, that the last term in Eq.(5.124) is only present if the Schroedinger operators do have an explicit time dependence, a case which is beyond the scope of this class.